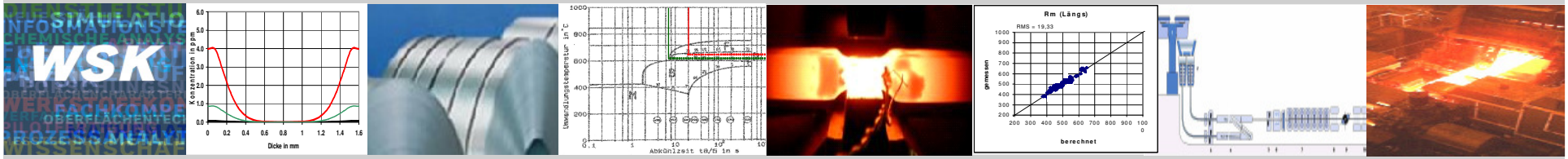
Using Computational Thermochemistry in a Steelmaking Enviroment



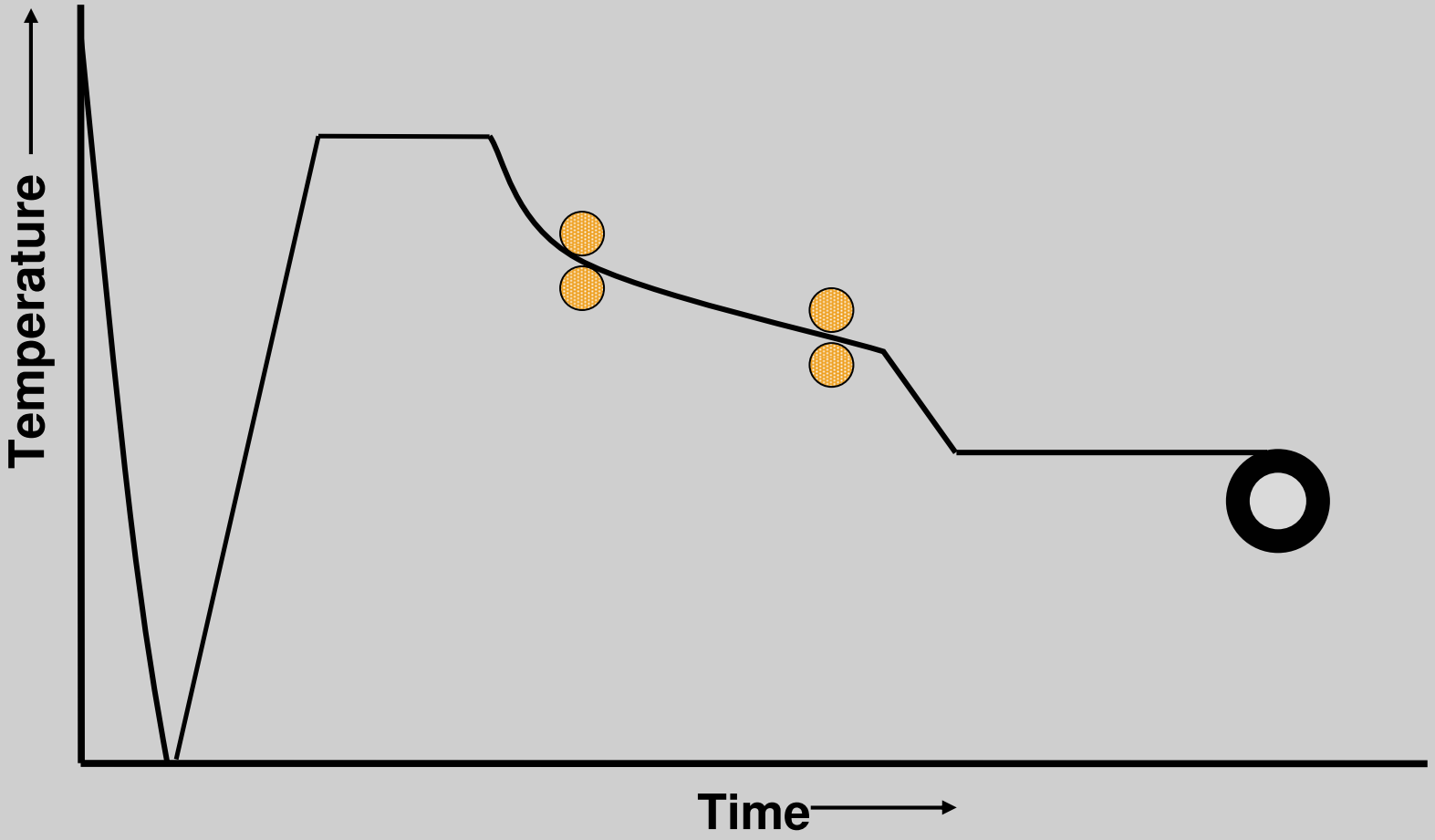
R. Großterlinden

GTT-Workshop, 4. – 6. Juni 2008

Using Computational Thermochemistry in a Steelmaking Enviroment

- Influence of preheating temperature on elements in solution
- Influence of traces of Ti on the solubility of Nb(C,N)
- Interaction between Ti4S2C2 and TiS in IF steels
- Bake Hardening in steels
- Thermodynamical calculations for microstructure simulation models
- Influence of carbone on hot forming properties
- c_p and H in thermal calculations

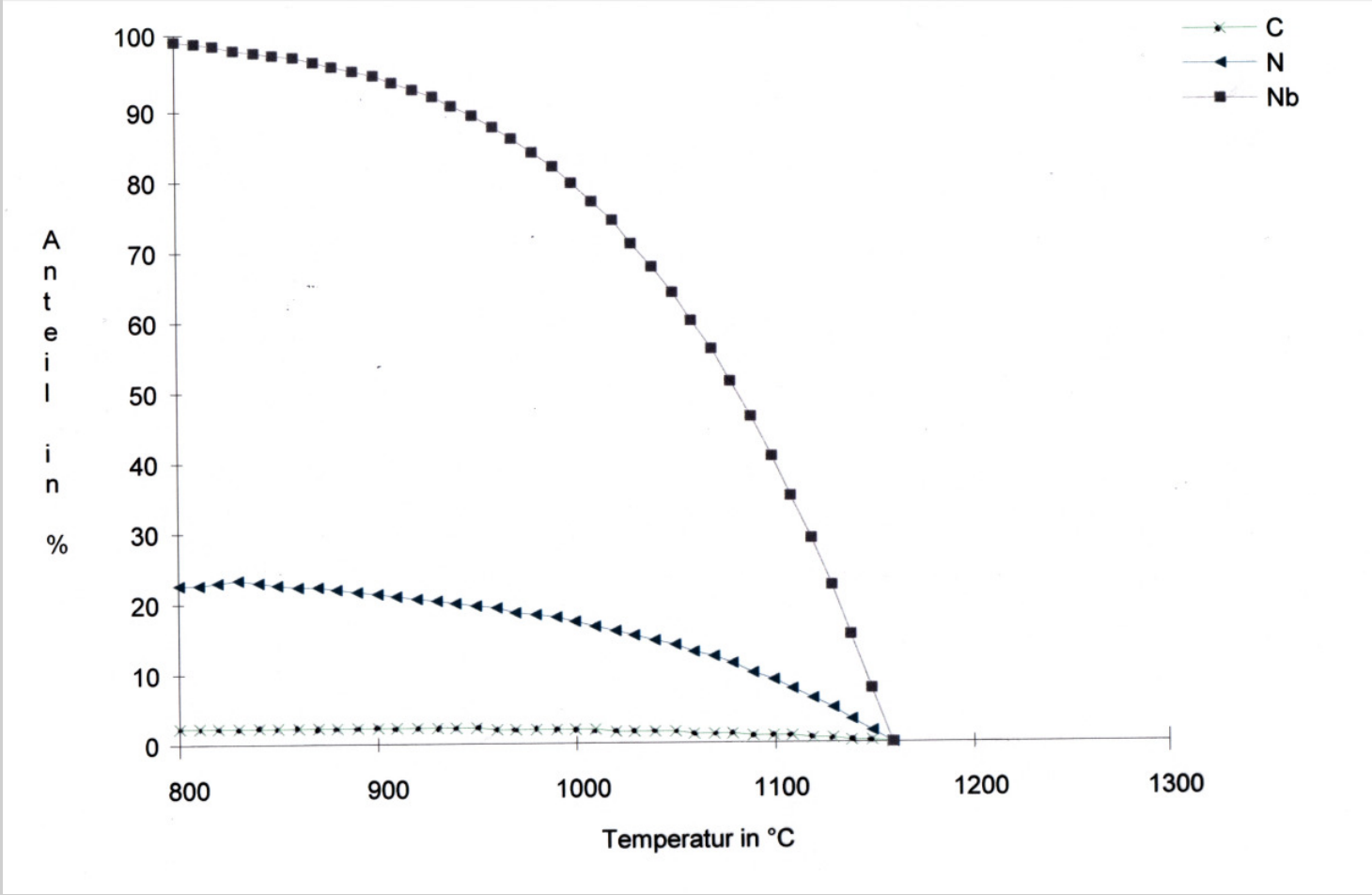
Pattern of Conventional Production of Hot Strip



Steel with 0,034%Nb without Ti

precipitated amout in % of the total content

(0,13%C; 0,04%Cr; 1,45%Mn; 0,0065%N; 0,034%Nb; 0,004%S; 0,035%Si)

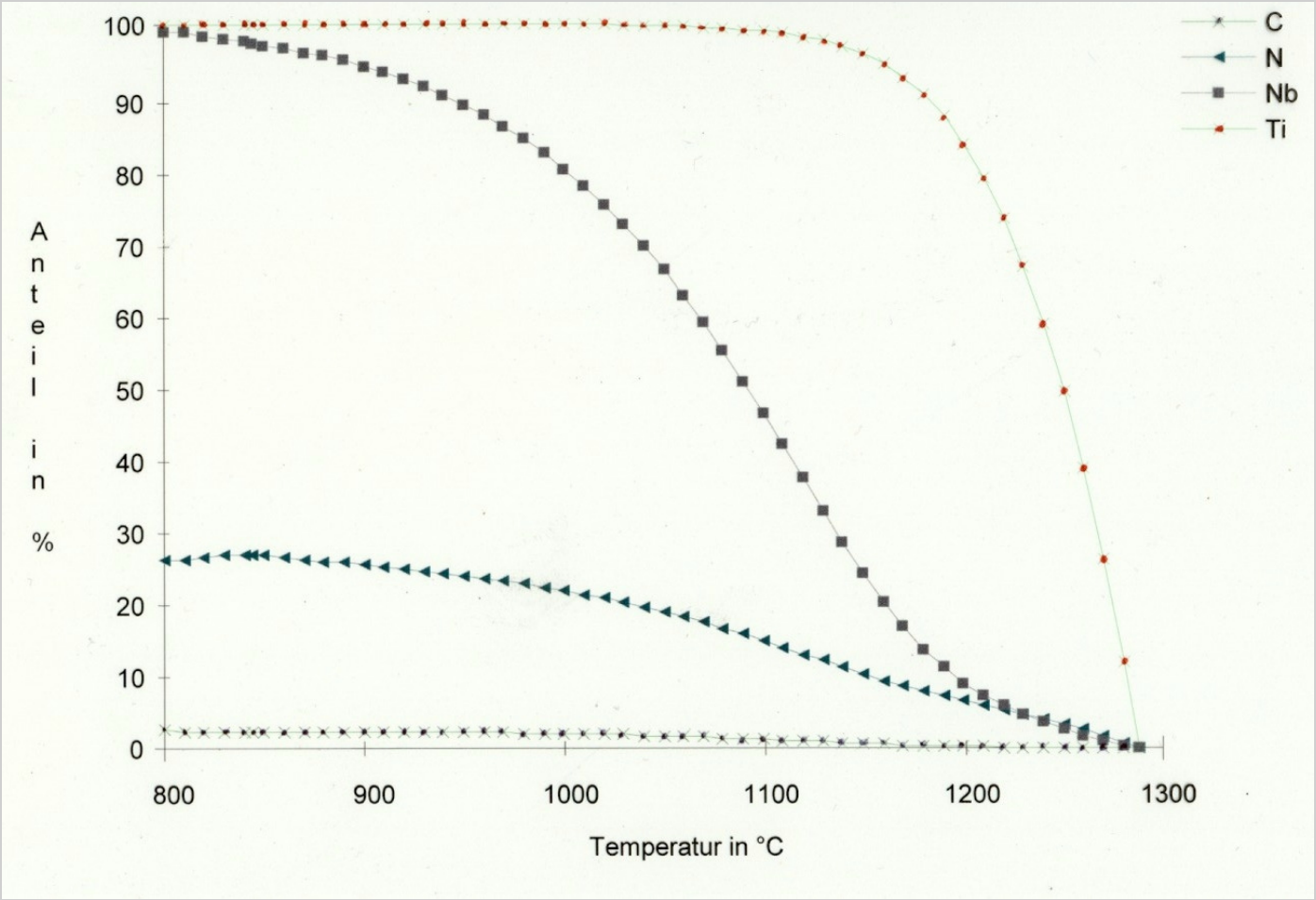


ThyssenKrupp Steel

Steel with 0,034%Nb and with 13 ppm Ti

precipitated amout in % of the total content

(0,13%C; 0,04%Cr; 1,45%Mn; 0,0065%N; 0,034%Nb; 0,004%S; 0,035%Si; 0.0013%Ti)



ThyssenKrupp Steel

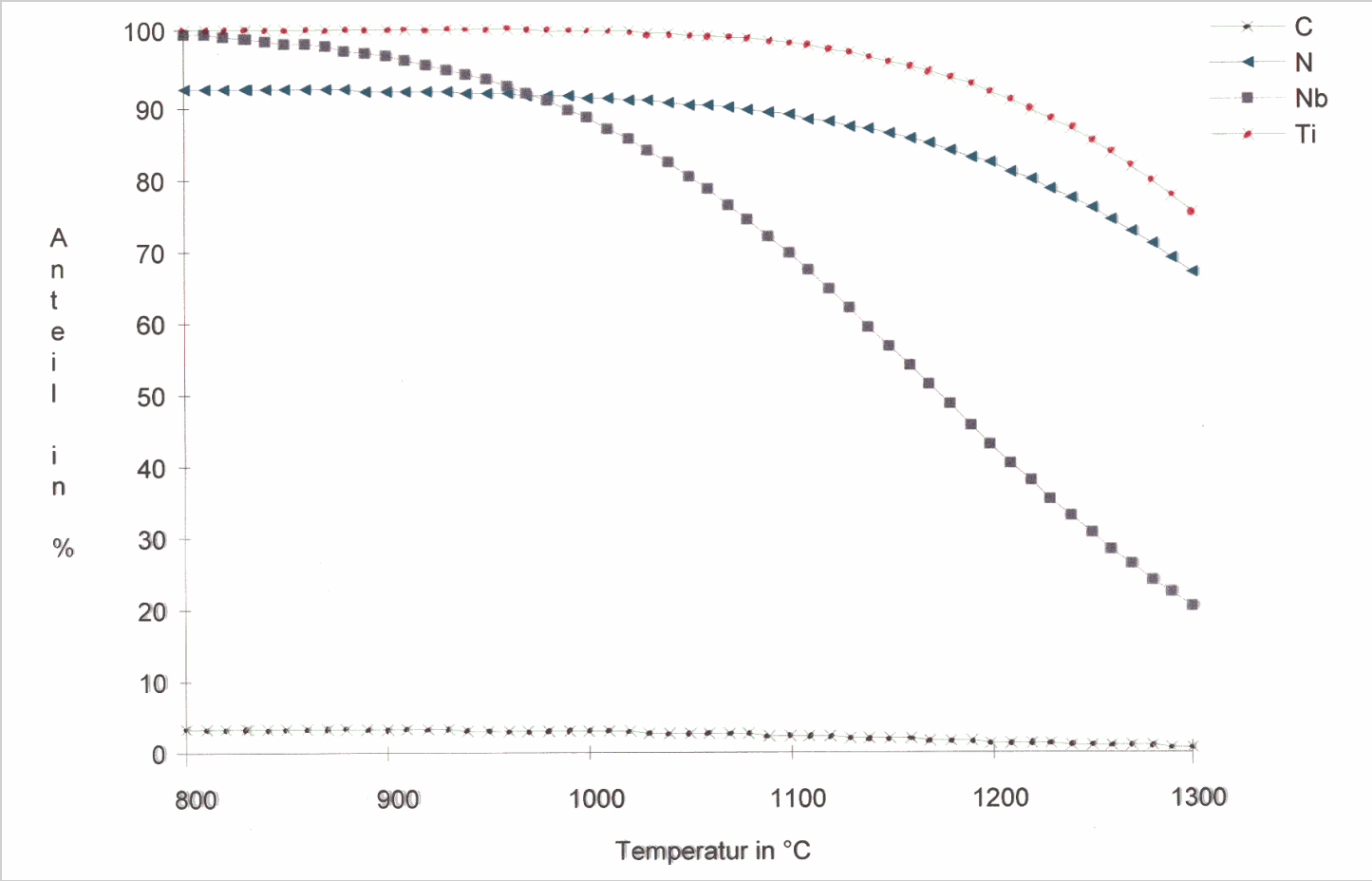
Free Energy

$$G = H - TS$$

Steel with 0,034%Nb and with 200 ppm Ti

precipitated amout in % of the total content

(0,13%C; 0,04%Cr; 1,45%Mn; 0,0065%N; 0,034%Nb; 0,004%S; 0,035%Si; 0.0200%Ti)

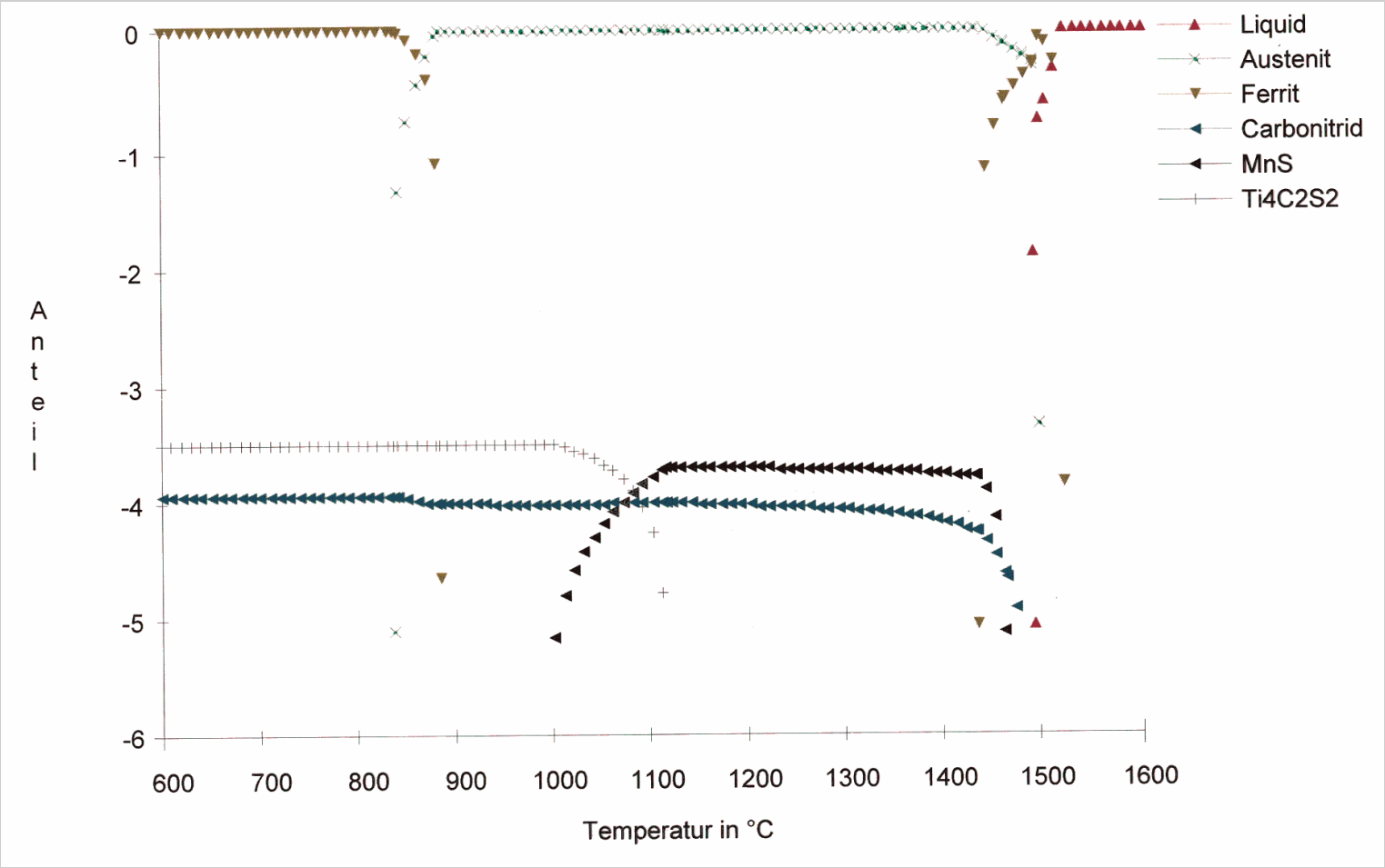


ThyssenKrupp Steel

Ti – Nb – Mn Steel

Amount of stable phases, logarithmic scale

(0,003%C; 1,5%Mn; 0,002%N; 0,02%Nb; 0,007%S; 0,06%Ti)

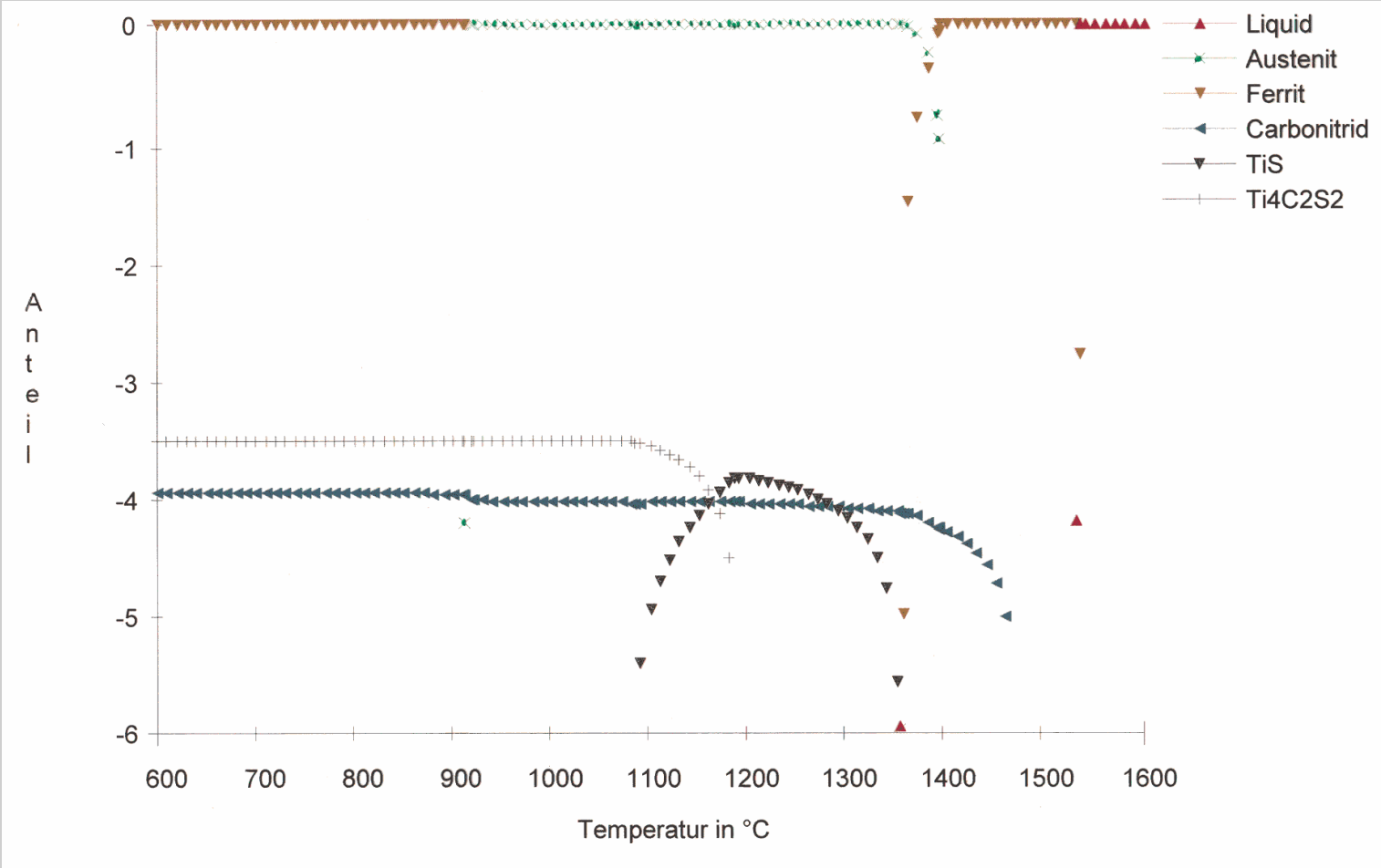


ThyssenKrupp Steel

Ti – Nb – Steel

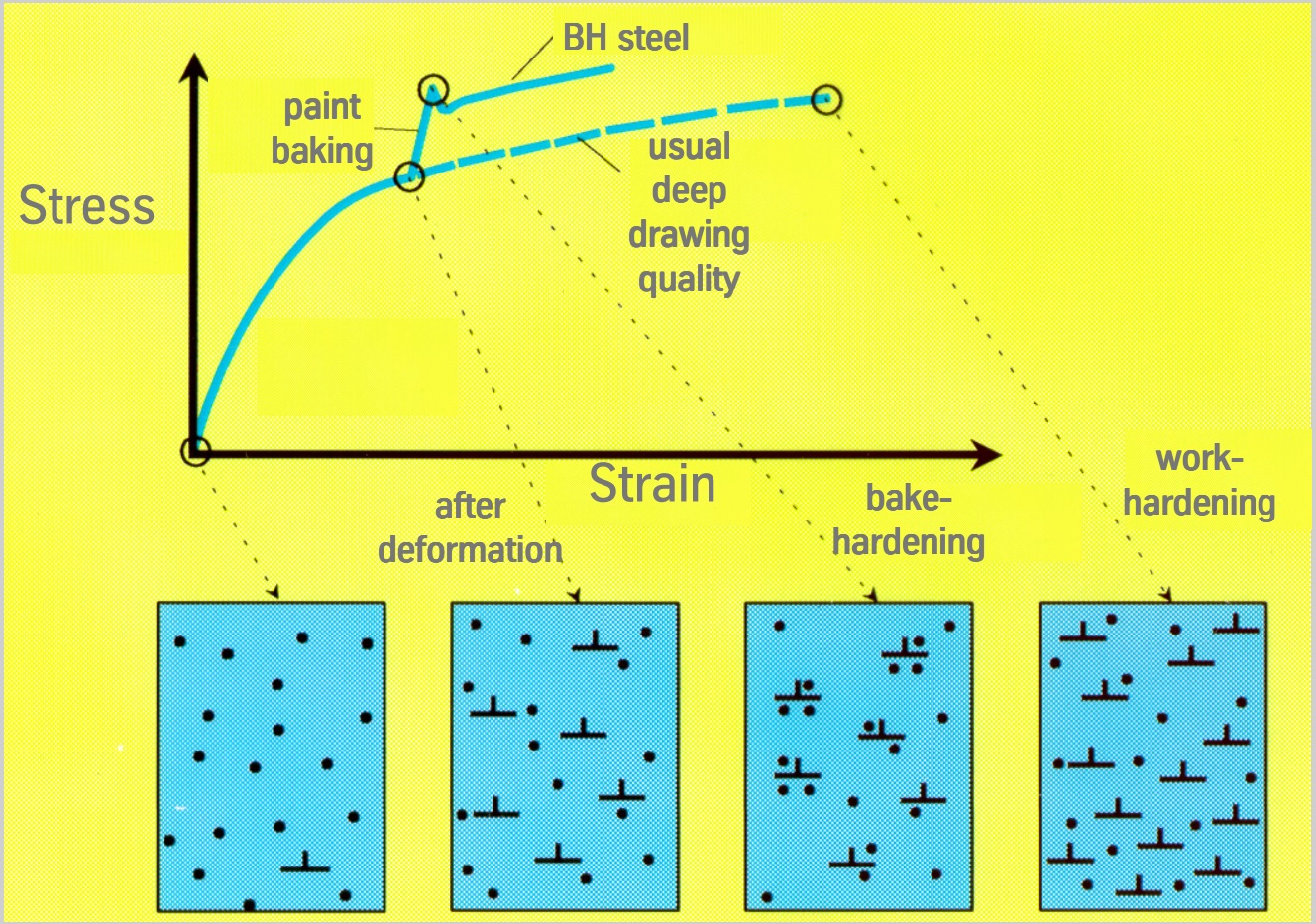
Amount of stable phases, logarithmic scale

(0,003%C; 0,1%Mn; 0,002%N; 0,02%Nb; 0,007%S; 0,06%Ti)

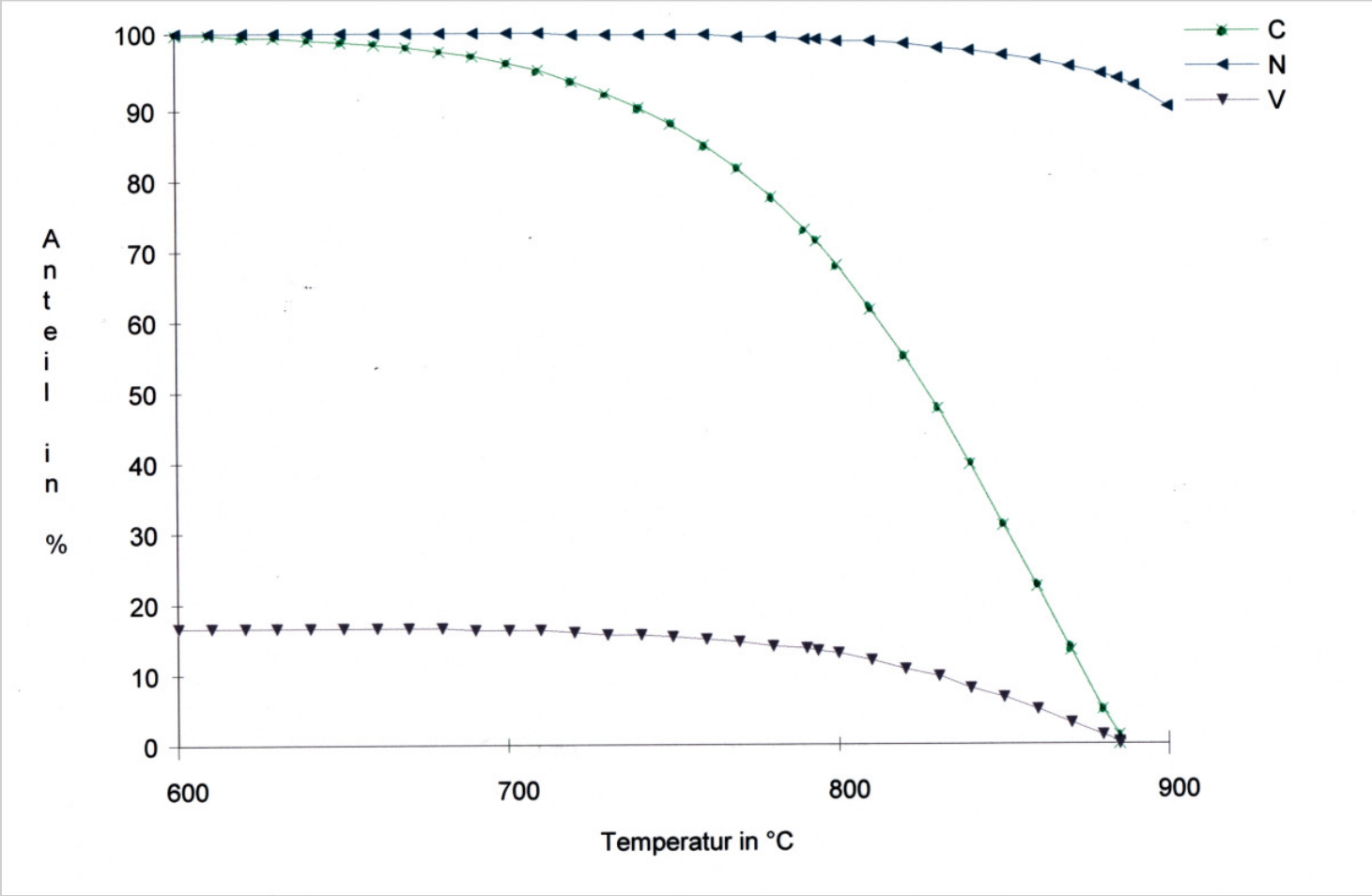


ThyssenKrupp Steel

Principles of Bake Hardening

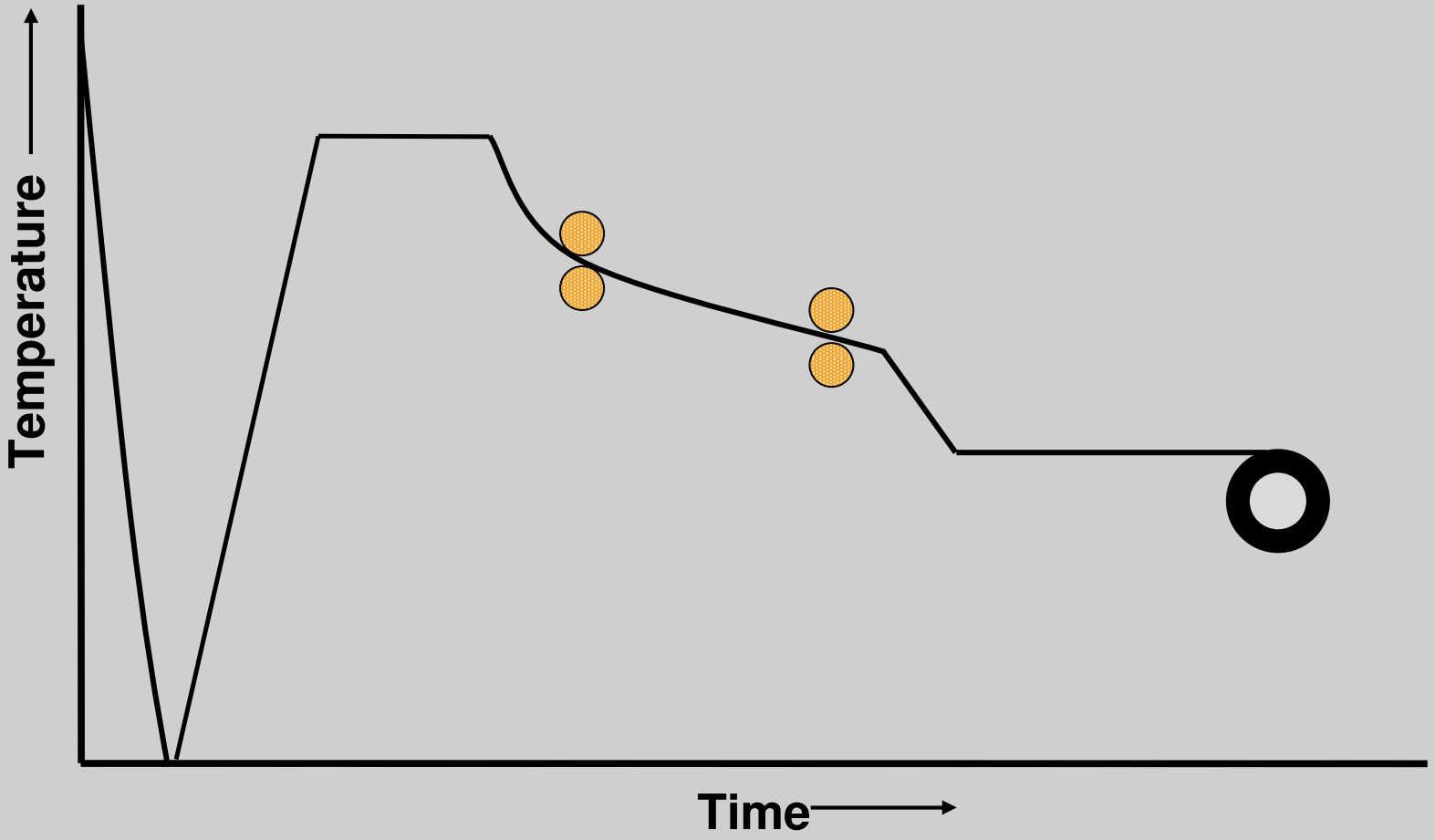


Precipitated Amounts in a V-Steel with 40ppm C

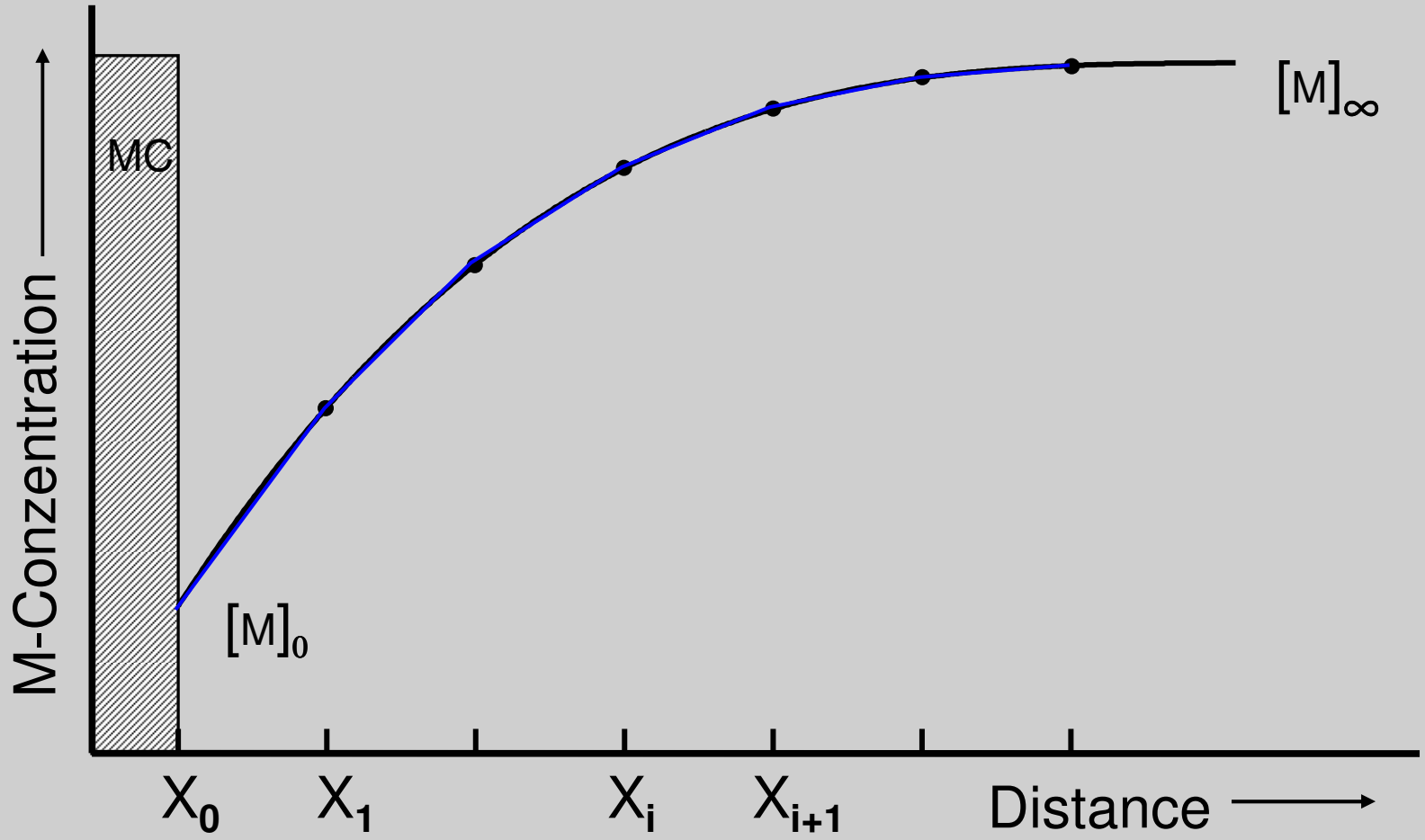


ThyssenKrupp Steel

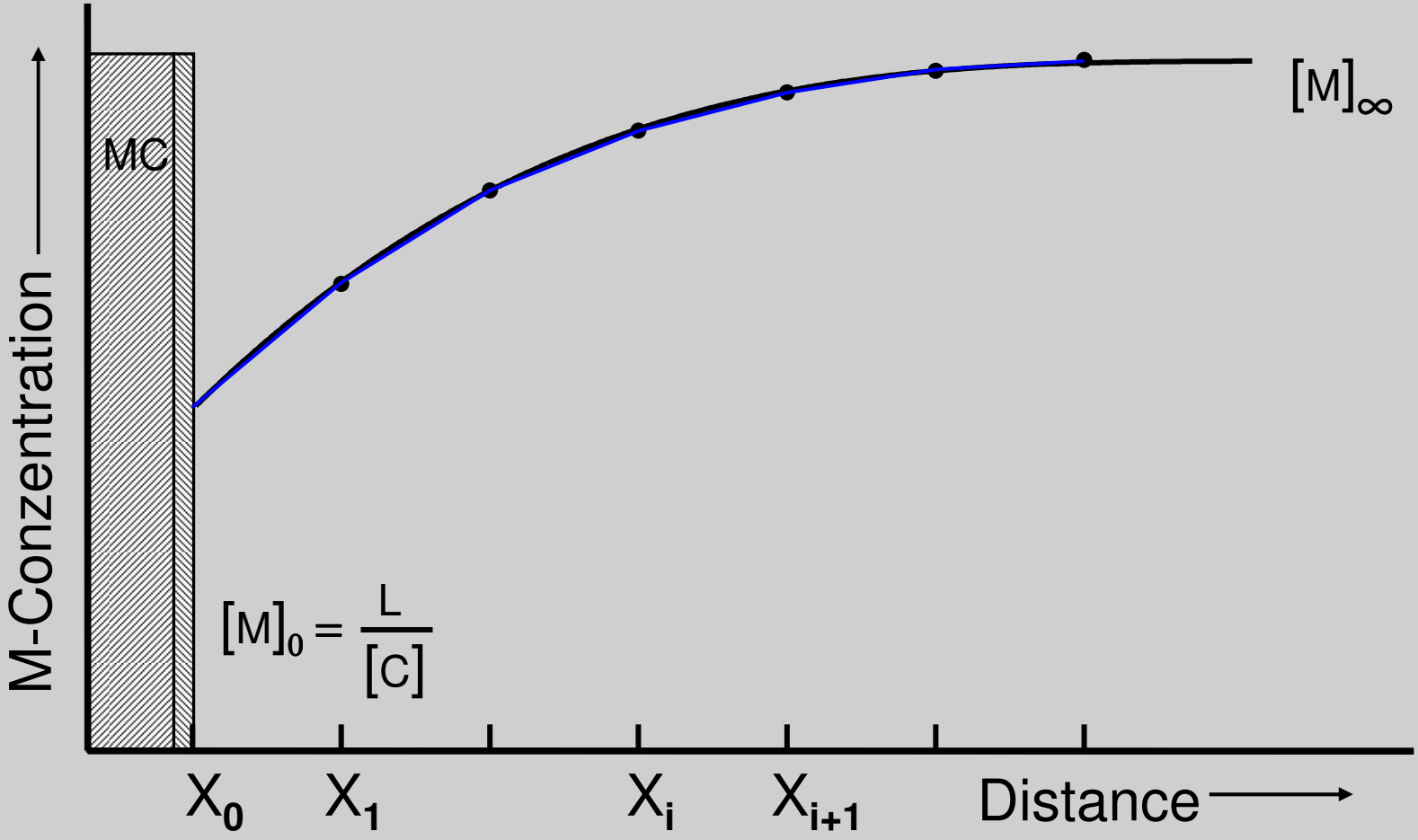
Pattern of Conventional Production of Hot Strip



Calculating Precipitation Kinetics using Finite Differences at Time = t_j



Calculating Precipitation Kinetics using Finite Differences at Time = t_{j+1}

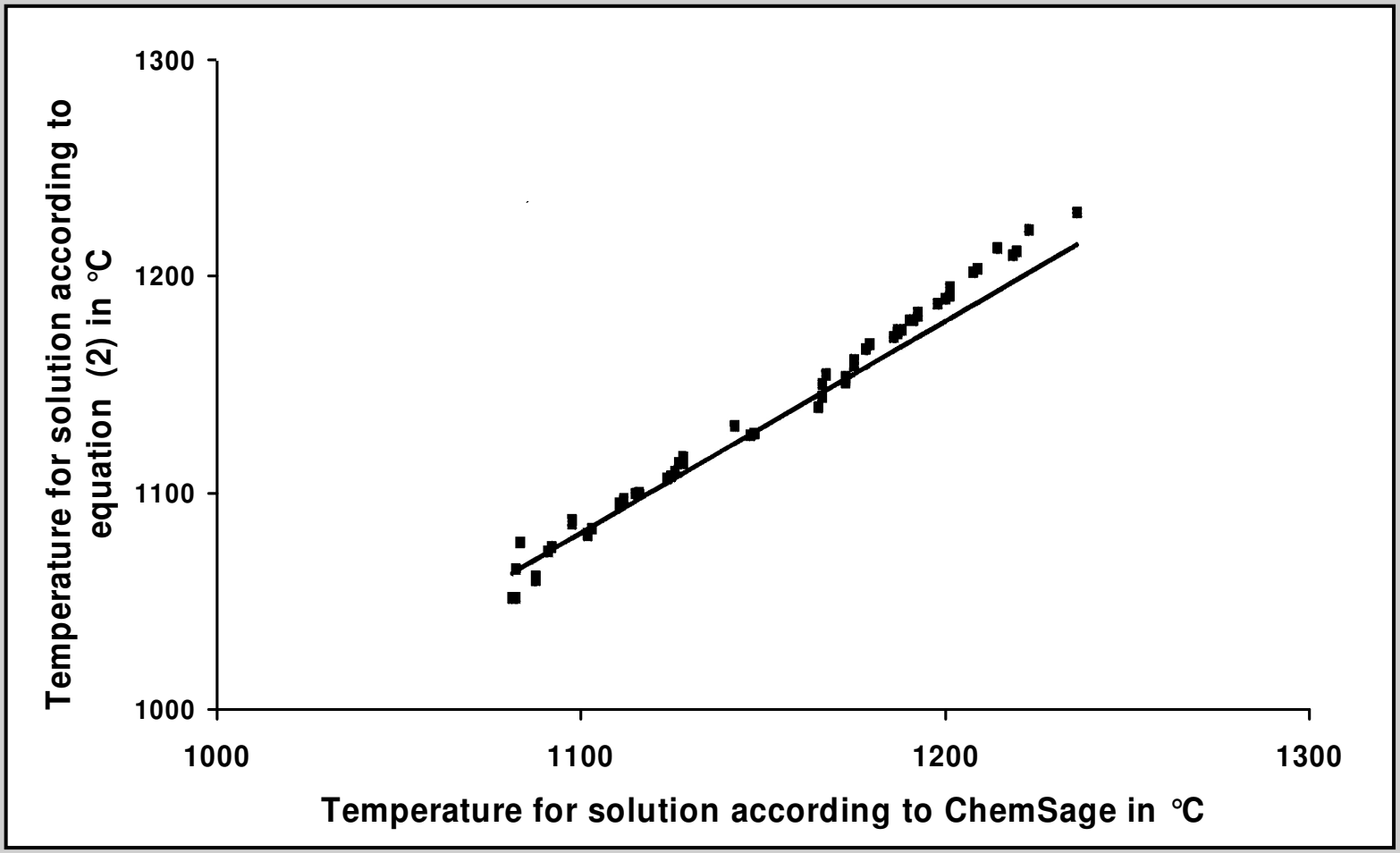


Equations for Solubility

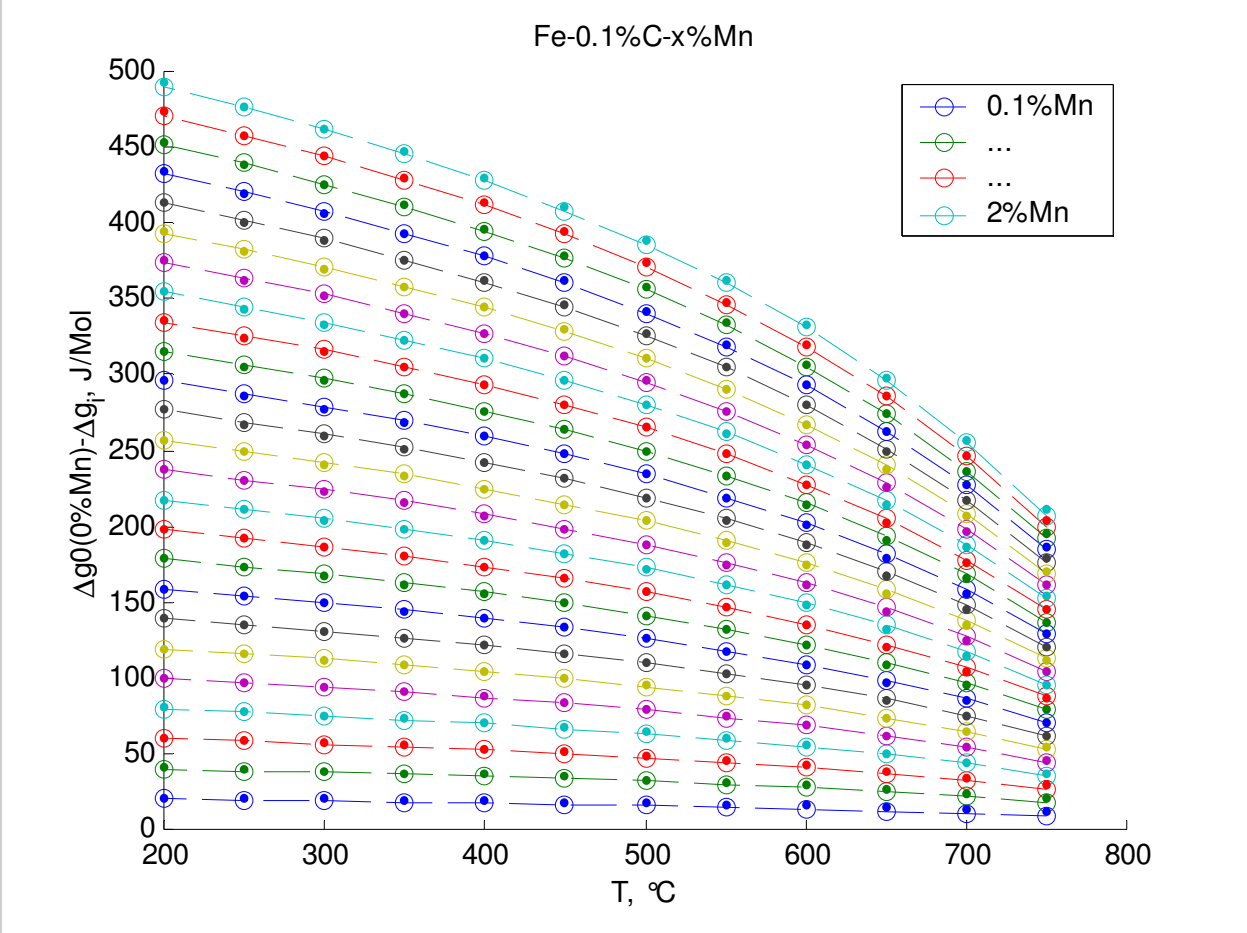
$$\lg\left(Nb \cdot N\right) = A - B/T \qquad 1)$$

$$\lg\left((b \cdot V + Nb) \cdot (N + a \cdot C)\right) = A_1 - B_1/T \qquad 2)$$

Fit of Equation 2

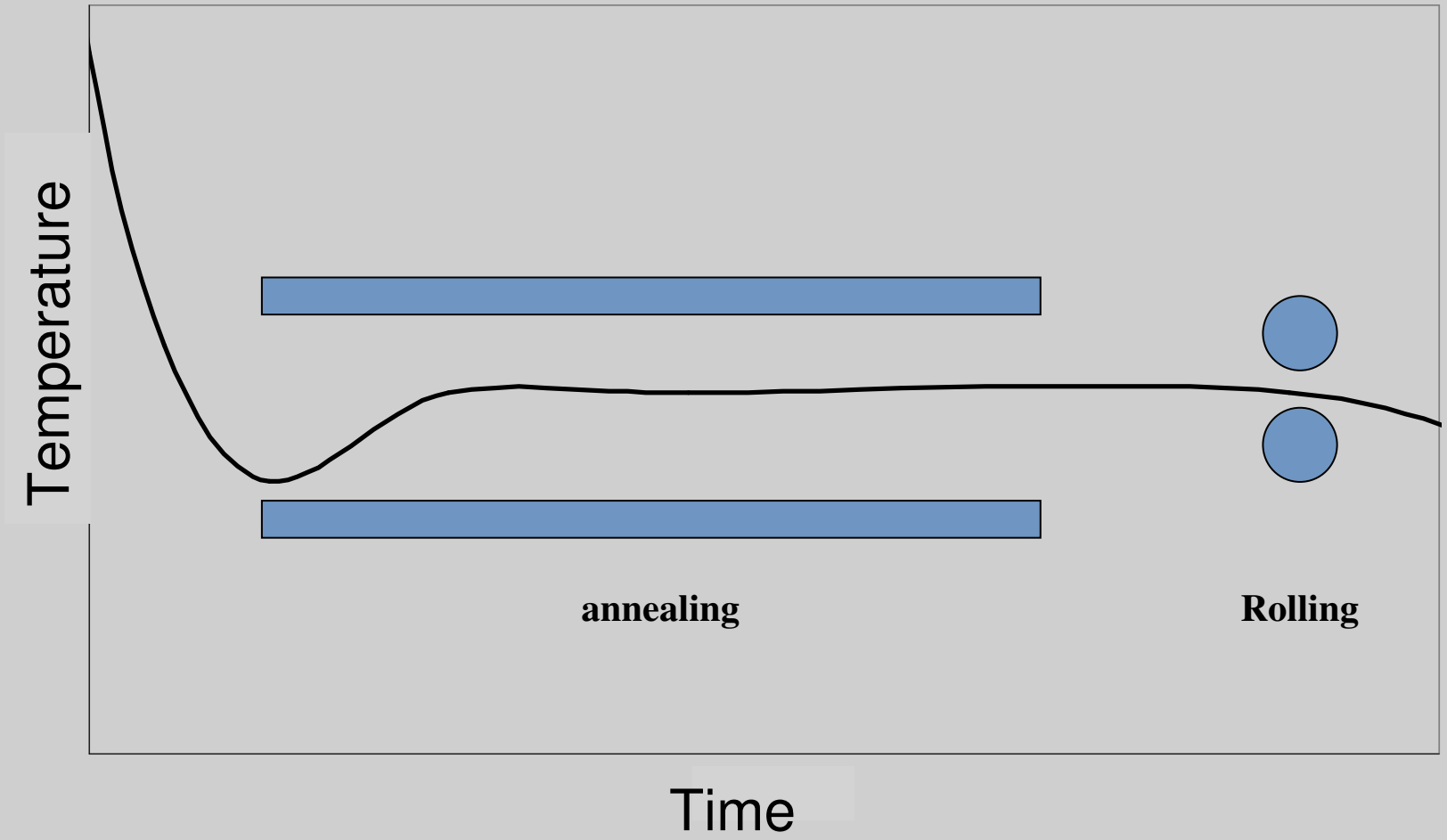


Differences of $\Delta g\ \gamma \rightarrow \alpha$ used in a Model for Transformation into Bainite



ThyssenKrupp Steel

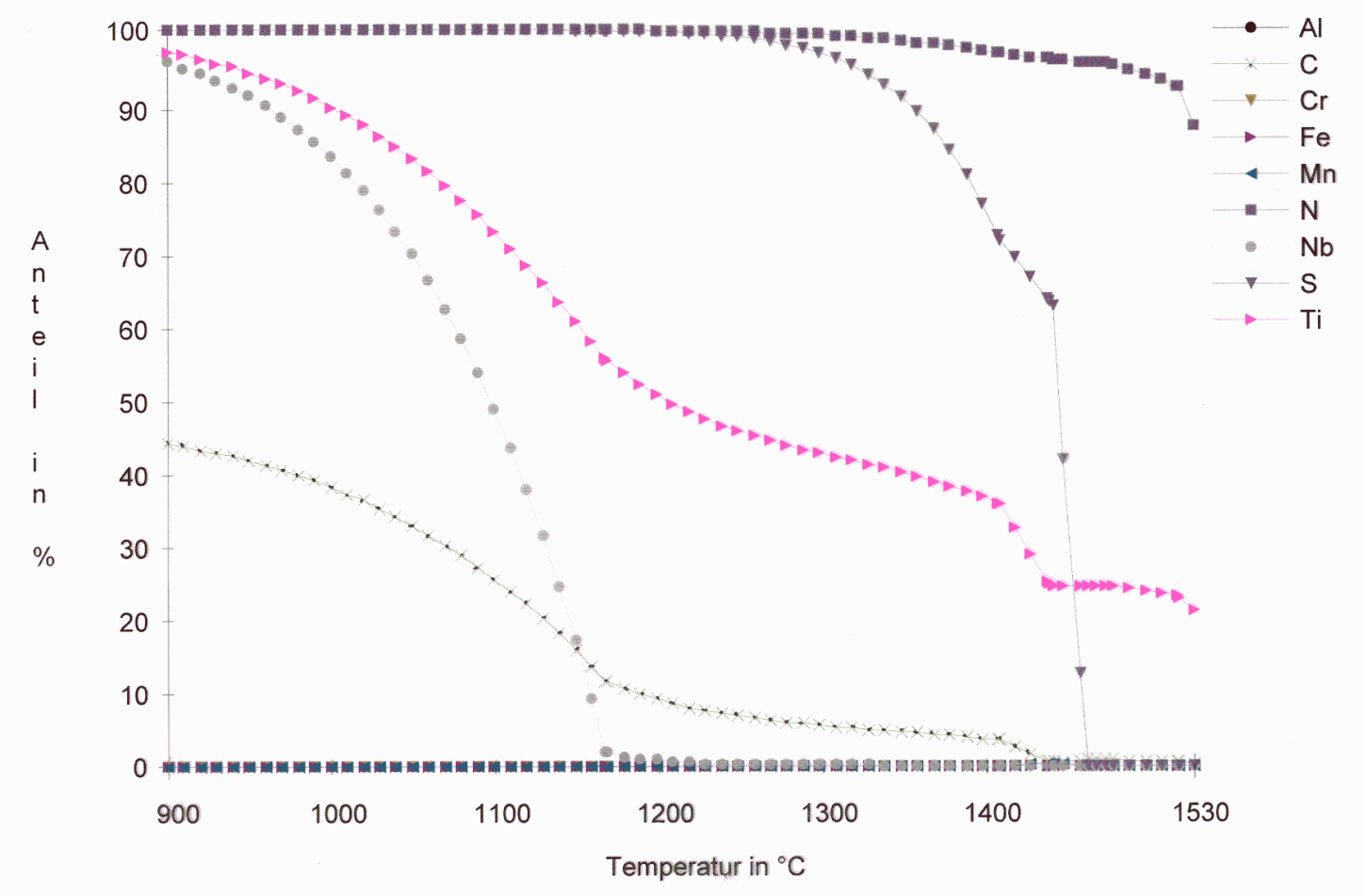
Temperature Cycle during Integrated Casting and Rolling



Steel 6

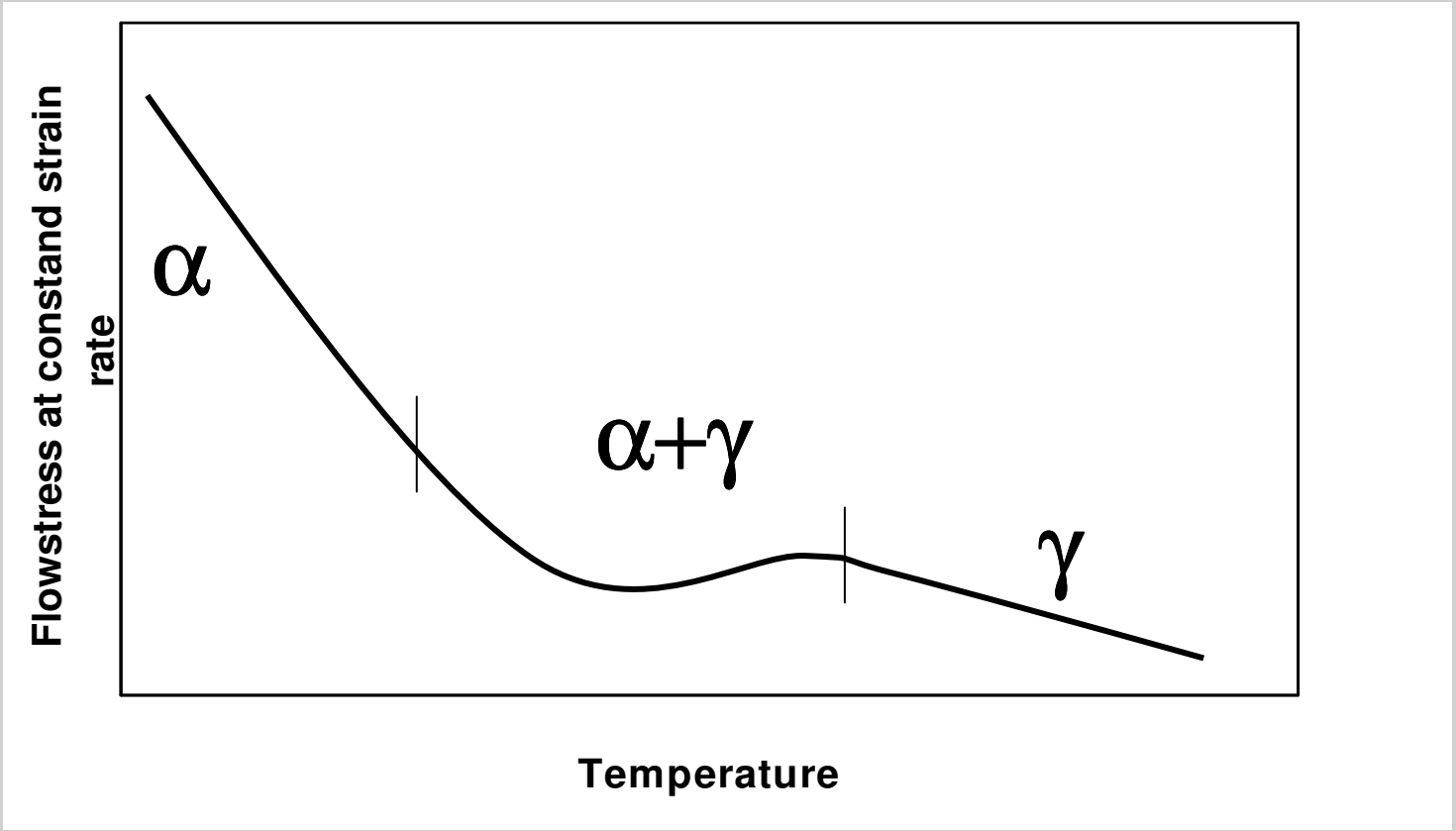
precipitated amout in % of the total content

(0,058C; 1,8%Mn; 0,03%Al; 0,06%Cr; 0,006%S; 0,06%Nb; 0,12%Ti)



ThyssenKrupp Steel

Elementary Diagram for the Dependency of Flow Stress on Temperature



Flow Model in the γ/α Region

$$k_f = A \cdot e^{m1 \cdot \vartheta} \cdot \vartheta^{m9} \cdot \varphi^{m2} \cdot e^{m4/\varphi} \cdot$$

$$\cdot (1+\varphi)^{m5 \cdot \vartheta} \cdot e^{m7 \cdot \varphi} \cdot \dot{\varphi}^{m3} \cdot \dot{\varphi}^{m8 \cdot \vartheta}$$

A, m1, ... m8 = const, ϑ = Temperature,

φ = Deformation, $\dot{\varphi}$ = Strainrate

$$K_{f\alpha/\gamma} = (\alpha \text{ Fraction}) \cdot K_{f\alpha} + (\gamma \text{ Fraction}) \cdot K_{f\gamma}$$

Influence of C Enrichement in Austenite

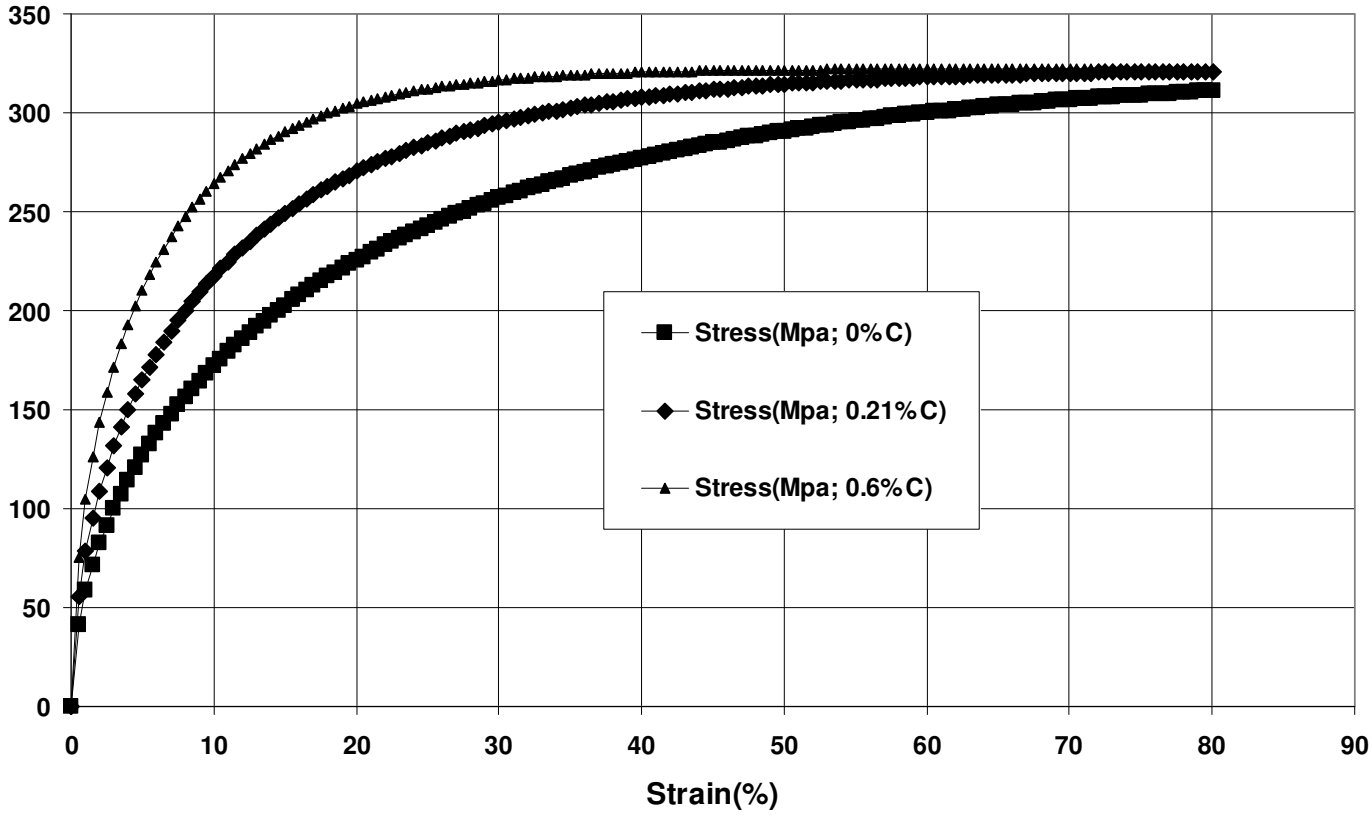
A. Schmitz und J. C. Herman: 1.st Int. Conf. on Modelling of Metal Rolling Processes, 1993, London

$$K_f = K_{f0}(1 - \exp(-r\varepsilon))^{0,5}$$

$$K_{f0} = 0,84(1 + 0,032\,Mn\,\%)\,\dot{\varepsilon}^{0,1} d_0^{-0,03} \exp(3537/T)$$

$$r = 112,7(1 + 3,88\,C\,\%)\,\dot{\varepsilon}^{-0,105}\, d_0 \exp(-2240/T)$$

Influence of C Enrichement in Austenite on Flowstress at 700 °C



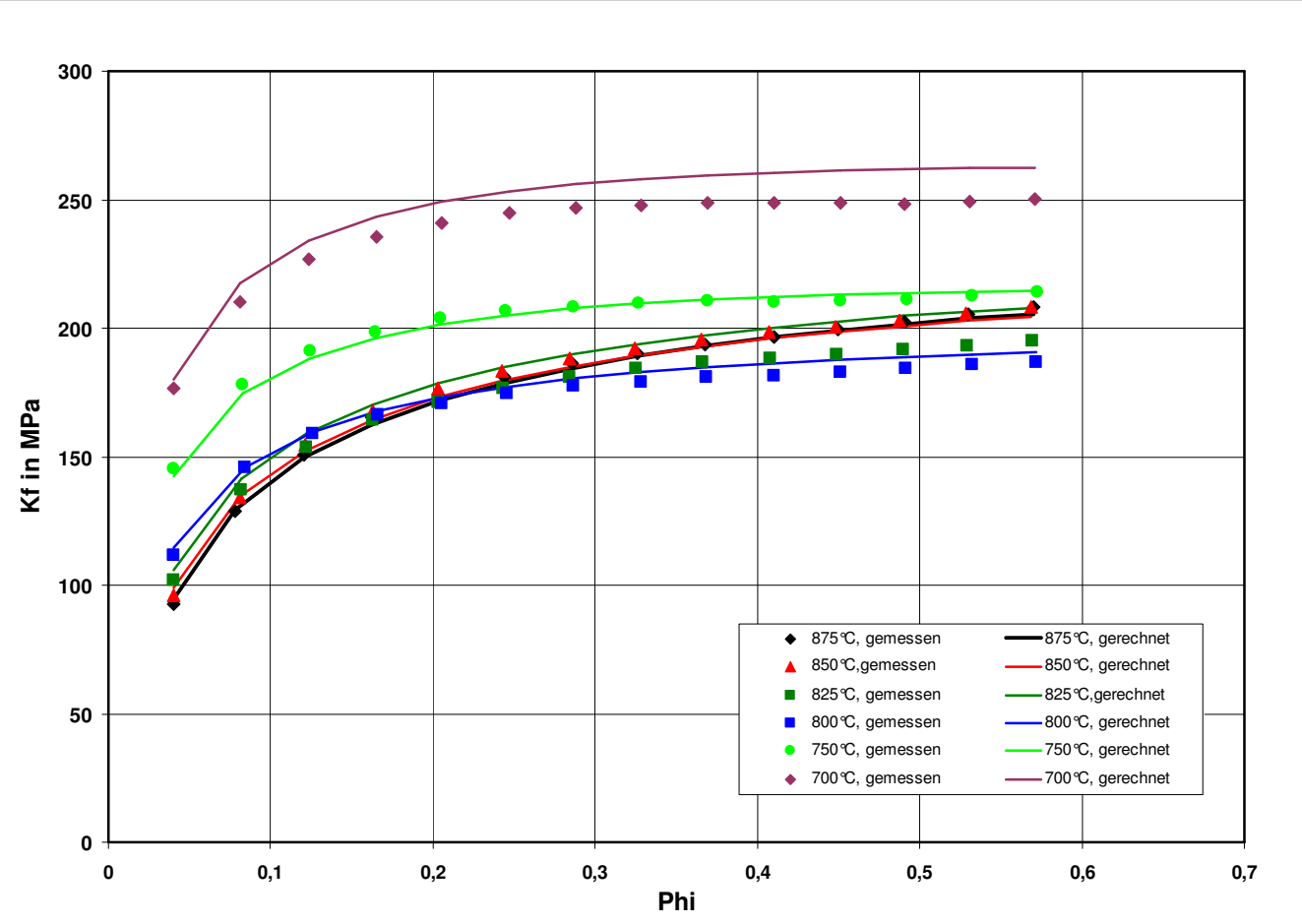
Part of the Result File for 740 °C from SteelMap

740°C

Mass fraction of the system components:

	GAS	BCC_A2#1	FCC_A1:Me#1	FCC_A1:Me#3
Al	3.6979E-09	1.6404E-04	7.7894E-05	3.2645E-11
C	1.2681E-07	***1.1206E-04***	5.1434E-03	1.1461E-01
Cr	1.5563E-07	1.0683E-04	1.9088E-04	5.3071E-04
Fe	5.4937E-05	9.7003E-01	9.5072E-01	7.6994E-04
Mn	9.9994E-01	1.0610E-02	2.8353E-02	2.2508E-03
Nb	1.5381E-27	5.9419E-08	7.3361E-08	8.8184E-01
Ni	3.0443E-09	1.3379E-04	3.2684E-04	6.1356E-07
S	3.5357E-07	1.3760E-09	5.0994E-10	8.7596E-14
Si	5.7273E-14	1.8847E-02	1.5189E-02	9.6818E-09

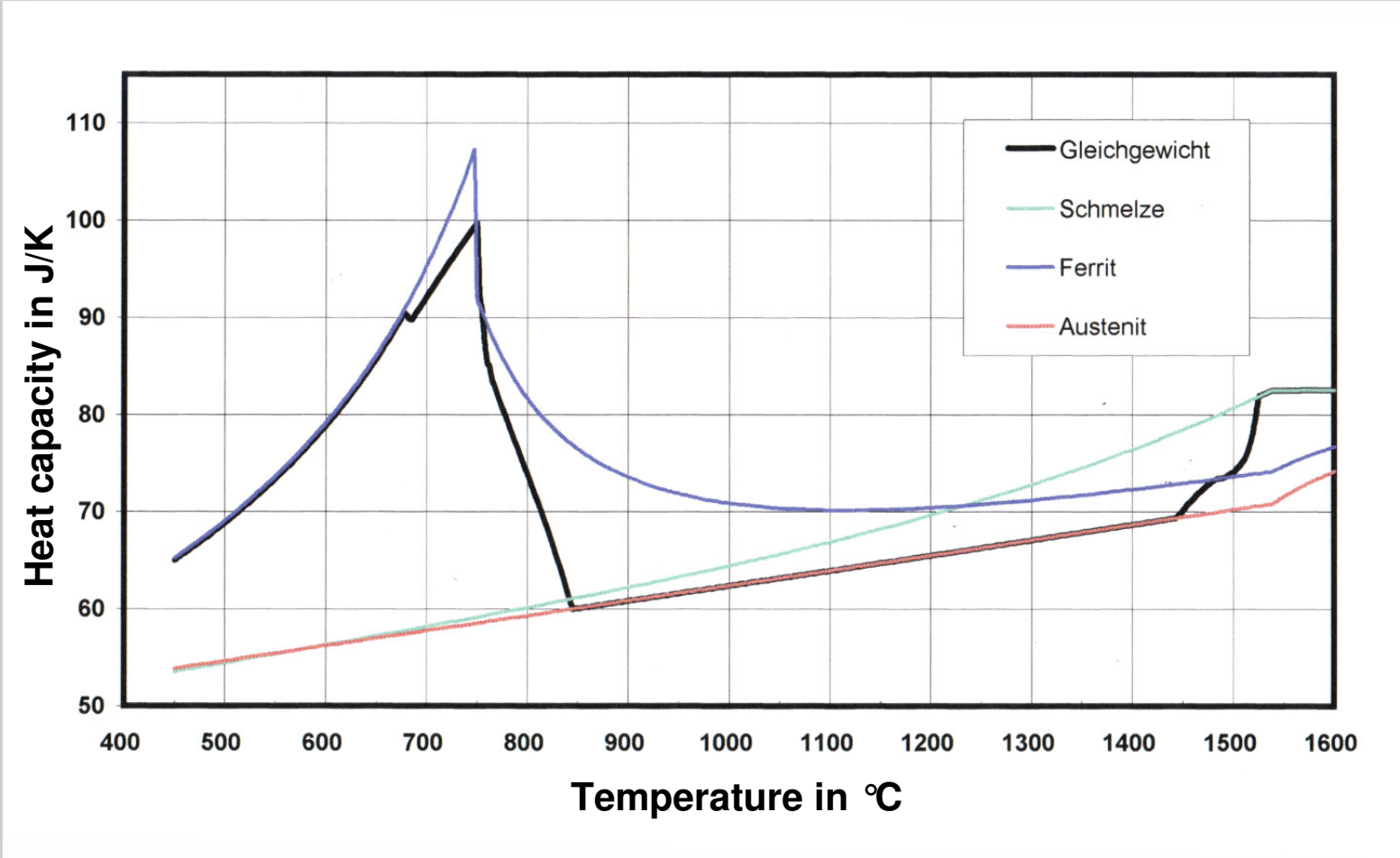
Measured and Calculated Flow Stress in the γ/α Region for φ· = 5/s



Thermal Conduction

$$c_p \cdot \rho \cdot \frac{\partial T}{\partial t} = \frac{\partial(\lambda \partial T)}{\partial x^2} + \Delta H \cdot \frac{\partial V}{\partial t}$$

Heat Capacity of 100 g Steel 7



ThyssenKrupp Steel

Enthalpie of 100g Steel 7